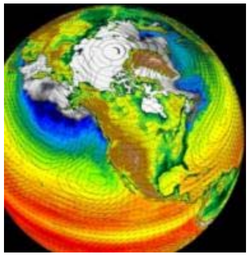
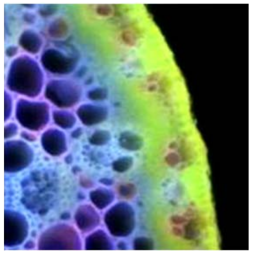
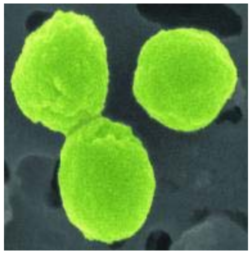


Biological and Environmental Research Workshop

Molecular Science Challenges

May 27-29, 2014

Co-organizers

James Liao
University of California, Los Angeles

Judy D. Wall
University of Missouri, Columbia

OBER Liaisons

Paul Bayer
Climate and Environmental
Science Division

Roland Hirsch
Biological Systems
Science Division

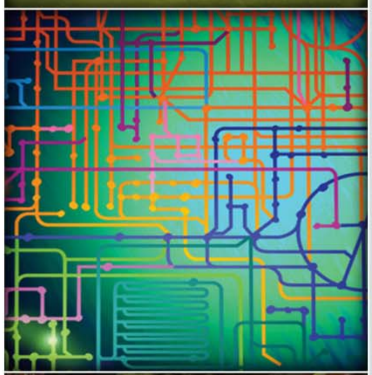
U.S. DEPARTMENT OF ENERGY

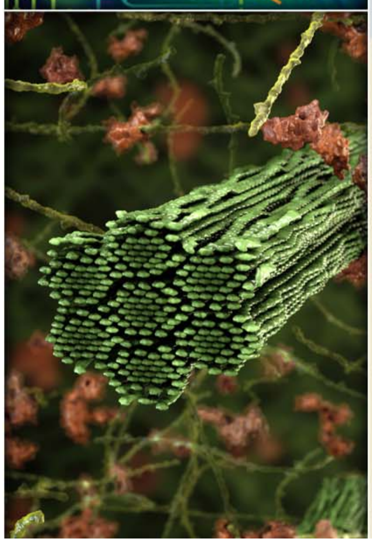
Office of Science

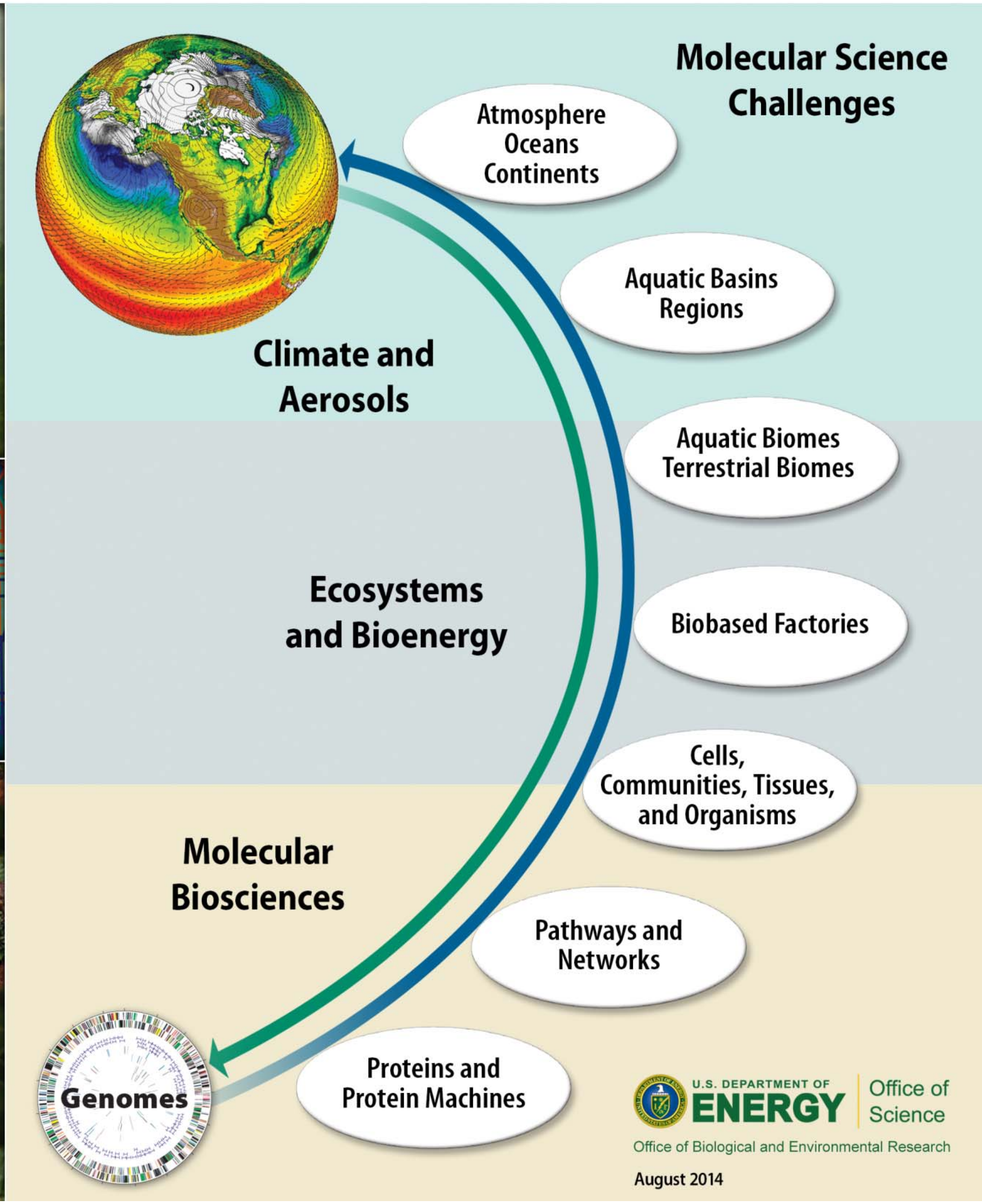
Office of Biological and Environmental Research

Workshop Charge

- **Understand the molecular systems and processes that underpin BER program goals.**
- **Integrate across breadth of spatial and temporal scales of the BER research areas.**
- **Take advantage of resources of the DOE National Labs and Facilities.**
- **Identify challenges and opportunities.**
- **Describe research pathways to overcome barriers in BER-relevant molecular science.**
- **Plan for a time horizon from *2014 through 2024.***







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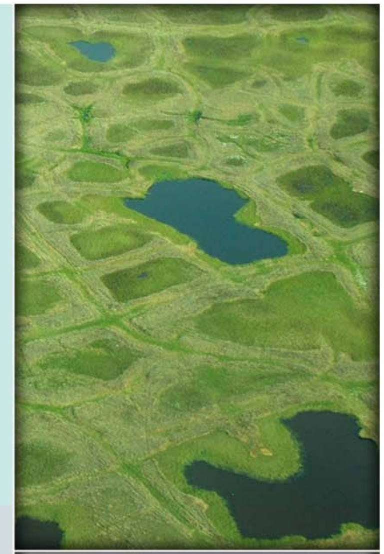
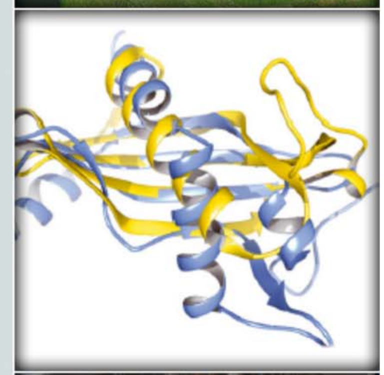
Office of Biological and Environmental Research

August 2014





Workshop Agenda

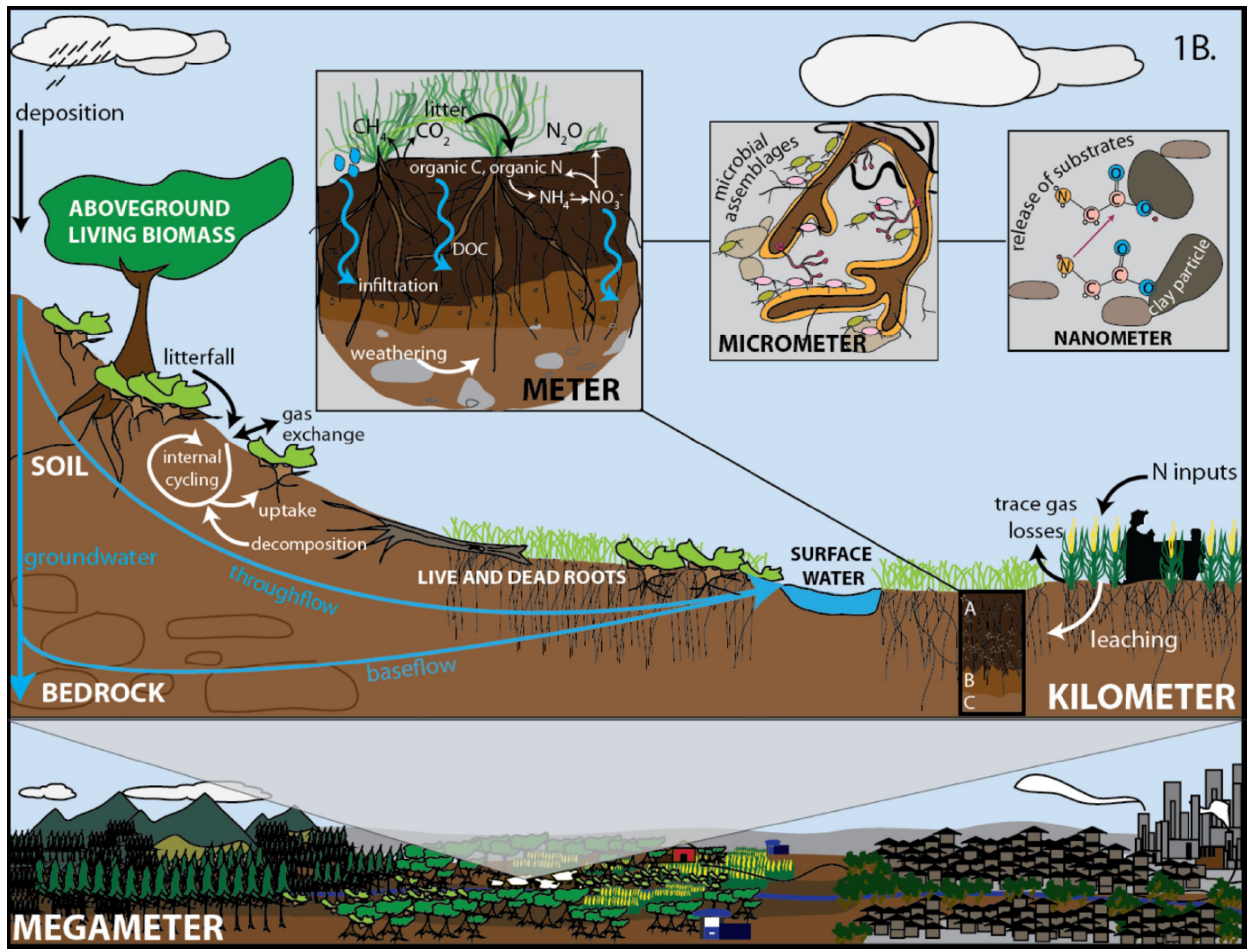
May 27-29, 2014	**One and one-half days**
Tuesday:	**Arrival and organizing dinner**
Wednesday:	**Welcome**
	Sharlene Weatherwax, Assoc. Director of Science for BER
	Todd Anderson, BSSD Director
	Gary Geernaert, CESD Director
	Keynote Address -- Jon Chorover
	Breakout sessions 1 and 2 and verbal reports
Thursday:	**Breakout session 3 and final verbal report**
	Writing session
	Concluding remarks.

Keynote Address
Carbon and Contaminants in the Critical Zone

Jon Chorover (and multiple collaborators)

Department of Soil, Water and Environmental Science

University of Arizona



Hinckley et al., 2014 *EOS* of AGU

Molecular Science Challenges Workshop

Breakout Groups

A) Atmosphere-Land Surface Interact

Vicki Grassian	Discussion Lead
Scott Bridgham	Rapporteur
Karl Booksh	
Rick Flagan	
Mary Gilles	
Sean McSweeney	
Theresa Windus	

B) Near Surface and Below-Surface Interactions

Michael Thomashow	Discussion Lead
John Bargar	Rapporteur
Kirsten Hofmockel	
Joel Kostka	
Jim Kubicki	
Al Valocchi	
Judy Wall	

C) Synthetic Science and Engineering

Norm Dovichi	Discussion Lead
Michael Crowley	Rapporteur
Michael Adams	
Jim Liao	
Steve Long (on phone)	
Jeremy Smith	
Ganesh Sriram	

Cross-cutting Themes

- Skilled workforce training needed
- Iterative interactions with modeling community
- Computational power- more accessible
- Expansion in observation capabilities
- Every scale shows heterogeneity
- Guidelines for parameterization of heterogeneous variables for predictive models

Atmosphere-Land Surface Interactions Involving Molecular Science

Decadal Vision

Determine how to meet the increasing need for energy without causing harm to the Earth's climate and environment.

Focus issues:

- ❑ **Exchange processes between land and atmosphere**
- ❑ **Aerosol links to radiative balance, cloud formation and precipitation**
- ❑ **Terrestrial ecosystem impacts from transfer of water, gases, organics and particles to and from the atmosphere**

Atmosphere-Land Surface Interactions Involving Molecular Science

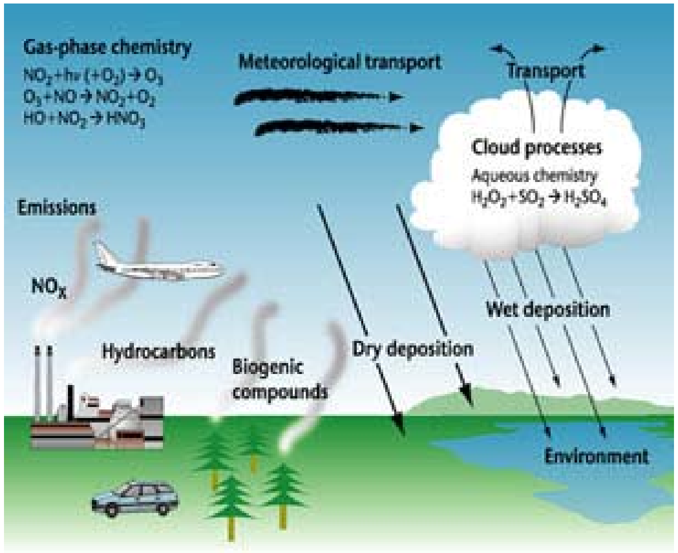
Decadal Thrusts

- **Exchange processes**

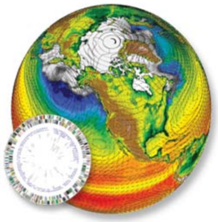
  Molecular Scale Data: Integrate molecular scale data into macro- and global-scale modeling to elucidate atmospheric impacts

  Biogenic and Anthropogenic Emissions: Identify and quantify the chemical and particulate emissions and depositions between land and atmosphere.

  Scale Interfaces: Are there unidentified phenomena operating across interfaces



http://www.metoffice.gov.uk/research/areas/chemistry-ecosystems/chemistry



Atmosphere-Land Surface Interactions Involving Molecular Science

Thrusts

Atmospheric aerosols

- ❑ **Modeling:** Obtain a global-level predictive ability a) for cloud formation and lifetime, b) for anthropogenic and biogenic emissions (gases and particles) and c) for the effects of clouds and emissions on the Earth's radiative balance.
- ❑ **Water Interactions:** Develop a theoretical understanding of water interactions with different types of aerosols
- ❑ **Biogenic Emissions:** Determine the mechanisms and rates of release of biogenic emissions from soil, natural waters, plant surfaces, and other sources through the action of microbes and other biological sources.

Terrestrial Ecosystem Impacts

- ❑ **Minerals and Organics**: Elucidate the molecular mechanisms of chemical and biological cycling of minerals and transformations of organic compounds.
- ❑ **Land Use Changes:** Ascertain the effects of land surface use changes on energy, particulate emissions and water transfers with the atmosphere.

Atmosphere-Land Surface Interactions Involving Molecular Science

Decadal Needs

Environmental Sensors:

Networks of sensors to probe the length and time scales that govern transport and reactions between air, soil, and water, and elucidate their effects on the development and growth of plants and microbes.

Sensor networks tunable to different resolutions to detect physical or chemical events.

Sensors low cost and long duration.

Analytical tools:

Analysis of natural samples at ultralow concentrations and low sample volumes

Computatiional power:

High speed distributive data archives

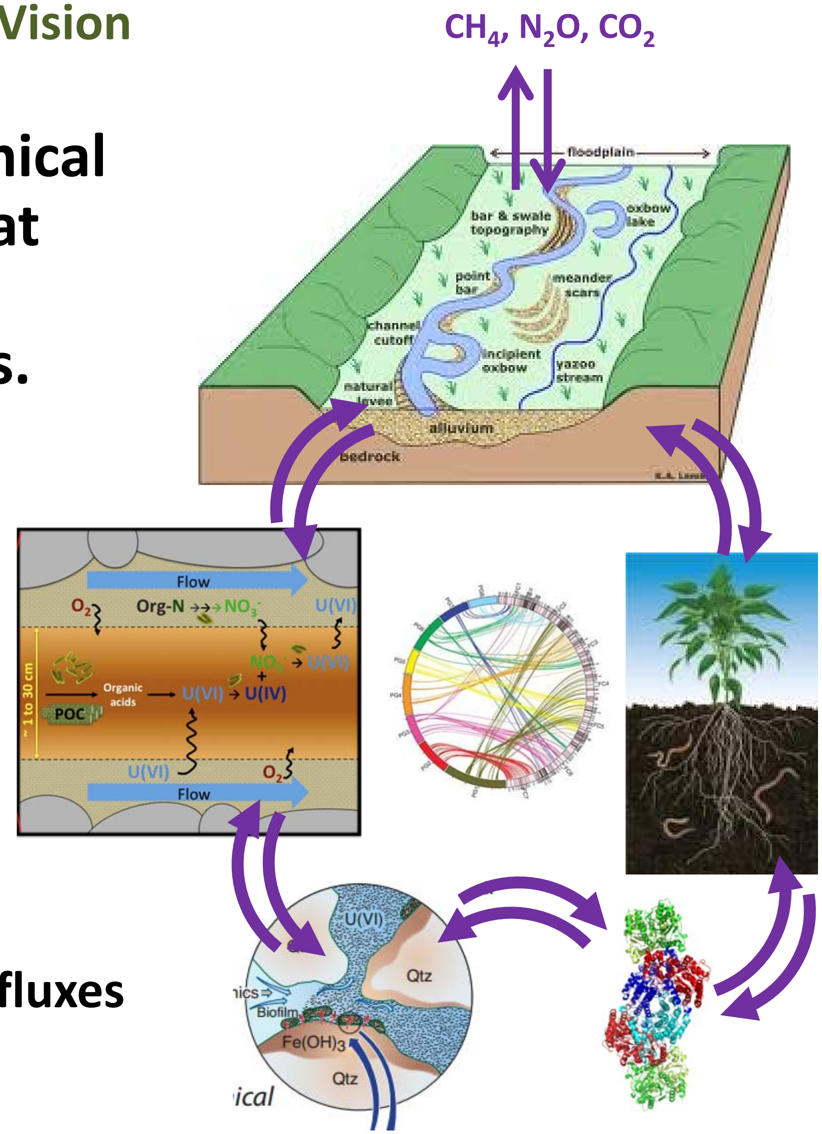
Workforce:

Multi-disciplinary training – DOE National Labs positioned well

Near-Surface and Below-Surface Interactions

Decadal Vision

Quantitatively understand biogeochemical *processes* and their *interdependences* at *molecular to ecosystem* scales under changing climate and land use patterns.



Must address:

- ❑ **Genes, plants, microorganisms, enzymes, sediments, soils, and water**
- ❑ **Molecular, pore, and meter scales**
- ❑ **Hot spots and hot moments**

Provides ability to predict:

- ❑ **Ecosystem-level nutrient and contaminant fluxes**
- ❑ **Ecosystem sustainability and tipping points**

Near-Surface and Below-Surface Interactions

Major Thrusts

- **Predict phenotype from genotype**

  Develop sensitive, non-invasive, high throughput technologies and methodologies to link genes with phenotypes in microorganisms and plants.

  Predict changes in microbial and plant population composition and structure caused by dynamic changes in the environment

- **Plant-microbe and microbe-microbe interaction mechanisms**

  Predict microbe-microbe and microbe-plant community interactions at molecular to millimeter scales.

- **Biogeochemistry in pores.**

  Determine the influence of pore size, bacterial, and mineral surfaces on the properties of water and aqueous reactions

  Establish electron shuttling/transfer mechanisms in complex natural systems

  Define enzyme functions at pore, ecosystem levels

- **Link subsystems and processes across scales to describe ecosystem behavior.**

  Develop techniques to detect, characterize, and monitor below-ground hot spots/moments

  Establish paradigms to scale molecular- and pore-scale processes to ecosystem, landscape scales

Near-Surface and Below-Surface Interactions

10-year Needs

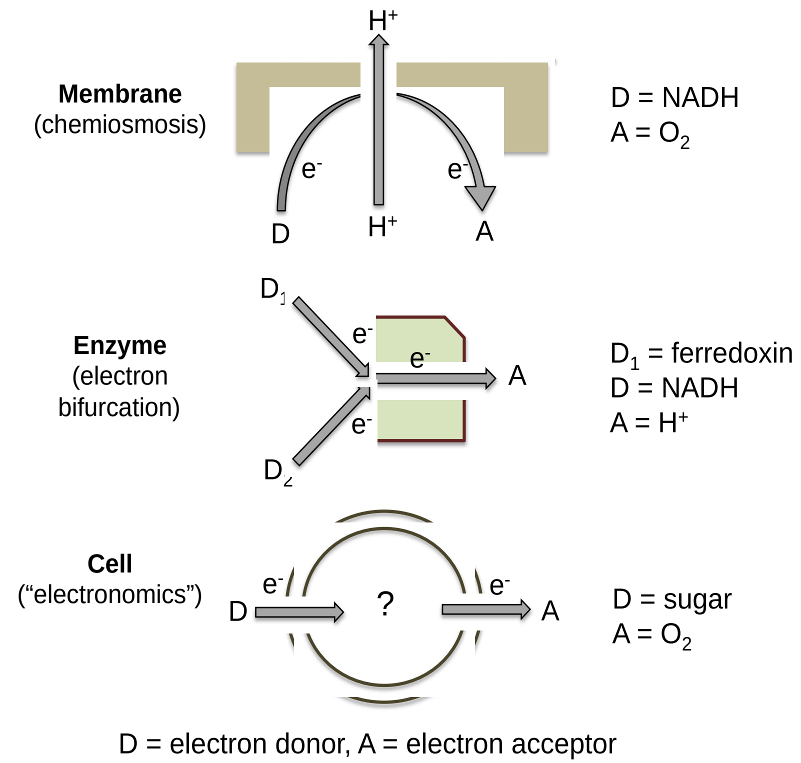
- **Imaging –** nm resolution, element speciation, ppm sensitivity, real time.
- **Spectroscopy –** Ultra-low volumes/masses (µg and µl), ultra-sensitive (sub-ppm, surfaces of minerals and microbial cells), high throughput, structure/composition, focus on pore scale: metals, organics, minerals, colloids, real time
- **Phenotype** - Non-invasive, high throughput, sensitive techniques for probing physiological responses.
- **Sensors** – Detect and monitor *in-situ* subsurface processes in real time at length scales of microns to meters (e.g., hot spots, hot moments, carbon content, solutes, functional genes)
- **Computational** – Expandable molecular modeling tools, more computational power
- **Thermodynamic/kinetic** – Constants needed for critical species

Synthetic Science and Engineering Involving Molecular Science

Decadal Vision

Newtonian Rules for Biology

Newton took on the challenge of formulating the fundamental laws of motion and converted the descriptive science to predictive physics. Currently the biological field can benefit from the discovery of “Newtonian-like” rules that underlie the interaction and evolution of biomolecules and processes.



Known and unknown principles of energy conversion

Synthetic Science and Engineering Involving Molecular Science

Thrusts

Electronomics Principles

- Management of energy transduction by cells engineered to produce a non-native function
- Impact of bifurcation of electrons on biofuel production

Multi-scale Three-dimensional View of Cell

- Three-dimensional time-resolved observation of biological cellular events to identify key players.
- Visualize, conceptualize and test molecular networks in time scale of relevance
- Observe and measure the impact of these molecular systems at successively linked system scales

Synthetic Science and Engineering Involving Molecular Science

10-year Needs

Knowledge needed to advance Newtonian biology

Multi-scale Three-dimensional View of Cell

Visualization tools for macromolecular structure and dynamics of the cell, positions of sub-cellular structures and distribution of metabolites and ions

Experimental and computational techniques capable of identifying individual macromolecular and small-molecule species in the cell

Time dependent three-dimensional view of the cell to follow evolution of systems

Molecular level computer simulation methods development

Computational methods to simulate, at the molecular level, the mechanisms of enzyme functions and macromolecular machines.

Multiscale computer simulation methods will lead to systems-level, prediction of the effects of molecular-level engineering

Appendix 3: MSCW Participants

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